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Bending of Nanoscale Thin Si Film Induced by Growth of Ge Islands: Hut vs. Dome

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ABSTRACT

We perform atomistic simulations to compute bending of freestanding nanoscale thin Si film induced by strained Ge islands. We show that a larger Ge dome island can induce smaller bending than a smaller hut island and explain the surprising experimental observation for growth of Ge islands on patterned silicon-on-insulator substrate (SOI) with Si template layer thinned down to nanometer scale. This counterintuitive bending behavior is caused by strain sharing between the film and the ultra thin substrate.

INTRODUCTION

In growth of coherent Ge film on Si(001), strain relaxation not only drives the initial island formation (2D to 3D transition) [1], but also induces the island shape transition from small-size pyramids (huts) having shallow (105) facets [1] to large-size domes having steeper (113) and (102) facets [1-3] with increasing Ge coverage. The bending of Si substrate induced by strained Ge islands can be used as a unique probe to monitor the island shape transition [4]. In general, when Ge grows on a thick Si substrate, the larger dome induces always a larger bending of Si substrate than does the smaller hut, as predicted by the classical Stoney's formula. However, when Ge is grown on SOI substrate with an ultra thin Si template layer, very recently, it has been observed that the larger dome induces a smaller bending than does a smaller hut, exactly the opposite of that on thick Si substrate [5].

In order to understand such a counterintuitive behavior, we have performed atomistic simulations to compute directly the bending of an ultra thin freestanding Si layer induced by both Ge hut and dome island. Our calculations confirm that the larger dome can indeed induce a smaller bending than does a smaller hut, when Si substrate thickness is reduced to be comparable to the height of Ge islands. We explain this bending behavior by large amount of strain sharing between the Ge island and Si film, i.e. the compliancy of the ultra thin Si film.

RESULTS AND DISCUSSION

In the experiment, the Si template layer in SOI is thinned down to ~10 nm, and Ge islands grow to a height ranging from 10~20 nm [5]. It has been observed that both dome and hut induce a very large localized bending underneath the individual island. The bending curvature induced by dome ($K \sim 5\times10^{-4}\ nm^{-1}$) is about one order of magnitude smaller than that by hut ($K \sim 3\times10^{-3}\ nm^{-1}$).

Continuum mechanics calculations [6] show that the magnitude of the large local bending approaches the maximum value of a freestanding Si film, which is assisted by the substantial local viscosity flow of SiO_2 underneath the Si. Quantitatively, the local bending mode can only occur when the thickness of substrate is reduced to be comparable to the height of islands in nanometer regime and those islands acting as nanostressors bend the Si thin film independently.

We therefore performed atomistic simulations to compute directly the bending of a freestanding ultra thin Si film induced by Ge islands, in order to better understand the experiments. The simulation cell contains a Ge island sitting on a Si freestanding layer. Initially, the Si layer is flat. The system is then relaxed by the total energy minimization until the force on each atom to be zero, reaching the final bent equilibrium structure. We calculate directly the

bending curvature of the equilibrium structure and compare the magnitude of bending induced by hut vs. dome. We use an empirical potential for Si and Ge, which gives a good description of elastic properties of Si and Ge [6]. Ideally, we would like to simulate the exact system as in experiment, but it will be computational too demanding. We therefore choose a much smaller model system with an island height of ~ 7Å for hut (Figure 1a) and ~14 Å for dome (Figure 1b) and a ~6 Å thick of Si film, to mimic closely the relative scales of experiment and to capture the physical condition that the thickness of Ge islands and Si film is comparable.

The atomic models of simulation systems containing a hut and a dome sitting on a Si(001) film, are shown Figures 1a and 1b, respectively. The hut, a pyramid, is square-based having four

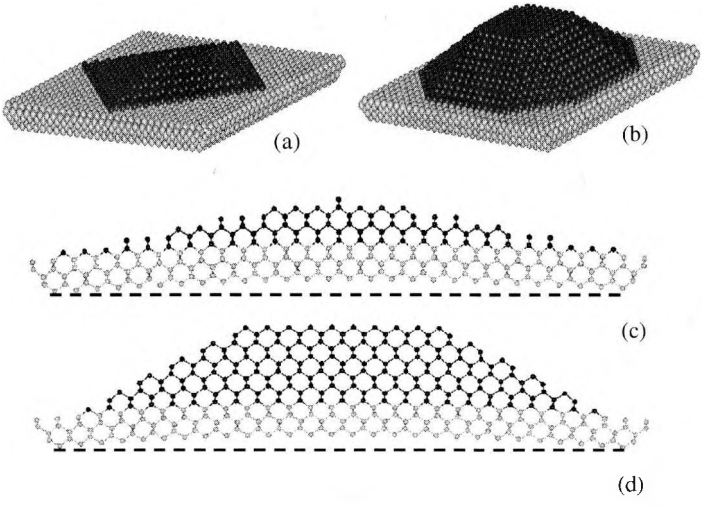

Figure 1. Atomic model of simulating a Ge island (black) sitting on a Si (001) substrate (grey). (a) Hut with bases along (100) directions. (b) Dome with bases in (100) and (110) directions. (c, d) The equilibrium bending structures along (110) direction for hut and dome, respectively. The larger dome induces a small bending than the smaller hut.

(105) side facets [1]; the dome is octagon-based having a (001) top facet, four (113) and four (102) side facets [2,3]. The island bases of the (113) facets are along the (110) direction, and those of the (102) facets are along the (100) direction. The lateral dimension of the Si substrate is chosen as 110 Å × 110 Å. These amount to ~5000 and ~8000 atoms for the hut (Figure 1a) and the dome system (Figure 1b), respectively.

Table 1 shows the average bending curvatures of the Si template calculated in the cross-sectional plane through the center of island along the island base in three high-symmetry (110), ($1\bar{1}0$) and (100) directions (see caption of Figure 1). Quantitatively, the larger dome induces consistently a smaller bending curvature than the smaller hut in all directions. For illustration, only the equilibrium bending structures along the (110) direction shown in Figure 1c and Figure 1d.

The counterintuitive bending behavior can be understood qualitatively as the following: When a strained film is grown on a substrate, it not only bends the substrate but also shares strain with the substrate. For a compressed film, it tends to uniformly expand the substrate. At low coverage, the film is much thinner than the substrate and its main effect is to bend the substrate slightly without expanding the substrate. Consequently, the bending curvature increases with increasing film thickness almost linearly. As the film coverage increases, the film tends to further expand the substrate, increasing the strain sharing between the two. Because the strain of the film is shared by substrate with uniform expansion, it effectively reduces the need to bend the substrate. Consequently, as the strain sharing increases with increasing film thickness, the bending slows down and starts to decrease after reaching the maximum, thereafter strain relaxation is largely achieved by uniform expansion.

Table 1. The average bending curvatures (in unit of 10^{-4} nm^{-1}) calculated in three high-symmetry (110), ($\bar{1}10$) and (100) directions along island base.

Island shape	Direction		
	(110)	($\bar{1}10$)	(100)
Hut	1.78	2.67	4.69
Dome	1.63	2.04	3.47

CONCLUSIONS

We have performed atomistic simulations to demonstrate the physical feasibility of an anomalous mechanical bending behavior: the lager dome induces a smaller bending than does a smaller hut, in good agreement with experiments. We explain such a counterintuitive behavior by the large strain sharing between the Ge island and Si substrate. When the Si substrate thickness reduced to be comparable to the height of Ge island in nanometer regime, where strain relaxation can be taken by strain sharing between film and substrate. Initially, the strain is relaxed by bending of substrate in low Ge coverage until reaching a maximum bending, thereafter strain sharing starts to be dominant by expanding the substrate with increasing the Ge coverage. This trend should be general true in any nanoscale films.

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